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Structural Studies of small molecules adsorbed in MOFs

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Adsorption of molecules in functionalized and high surface area microporous materials is of technological importance in a multitude of areas ranging from chemical separations to energy storage. Over the past several years we have focused our research efforts on understanding the properties of metal-organic frameworks (MOFs) and zeolites for storage and separations of industrially important small molecules such as hydrogen [1], oxygen [2], carbon dioxide [3], noble gases, and short chain organics. Besides the geometrical and porosity control in either class of materials, the properties of metal-organic frameworks can be tuned to optimize electrostatic interactions by exposing open metal cation sites. Here, we discuss the different requirements for performing these experiments at X-ray compared to neutron sources and reflect on the information potentially obtainable in both cases. The results illustrate the power, and limitations, of diffraction in elucidating many of the governing characteristics of these material properties and the interactions with the guest molecules.

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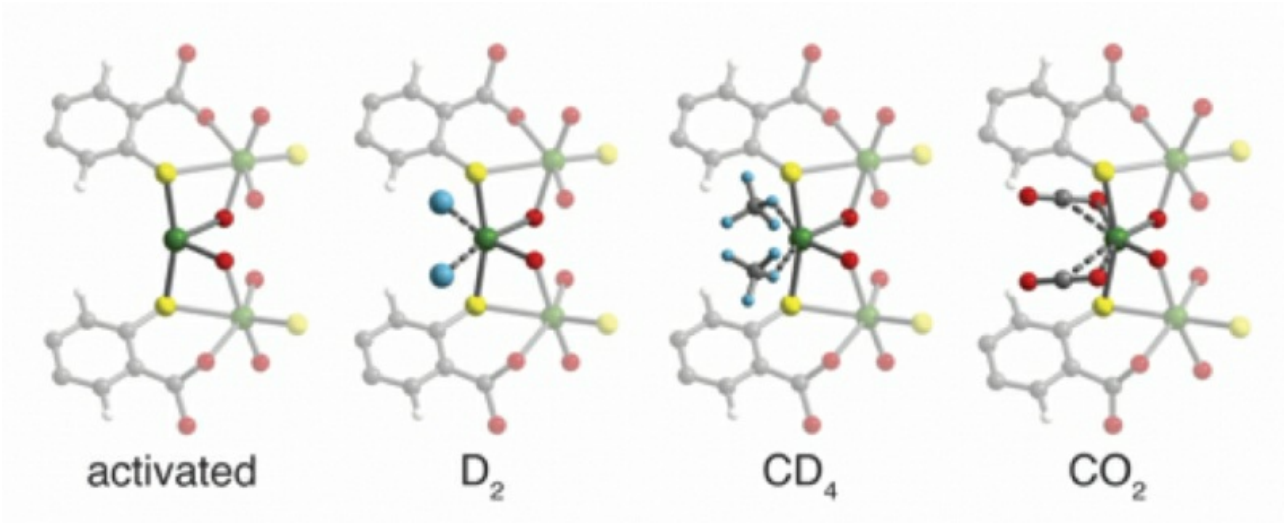

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